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# (2*E*)-3-(6-Methoxynaphthalen-2-yl)-1-[4-(methylsulfanyl)phenyl]prop-2-en-1-one

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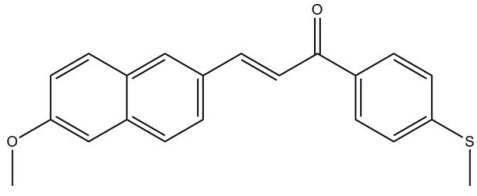
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.005 Å; $R$ factor = 0.055; $wR$ factor = 0.136; data-to-parameter ratio = 20.0.

The asymmetric unit of the title compound, $C_{21}H_{18}O_2S$, consists of two crystallographically independent molecules (*A* and *B*). The molecules exist in a *trans* conformation with respect to the central C=C bond. The naphthalene ring system makes dihedral angles of 51.62 (12) (molecule *A*) and 52.69 (12)° (molecule *B*) with the benzene ring. In molecule *A*, the prop-2-en-1-one group forms dihedral angles of 22.84 (15) and 29.02 (12)° with the adjacent naphthalene ring system and benzene ring, respectively, whereas the corresponding angles are 30.04 (12) and 23.33 (12)° in molecule *B*. In the crystal, molecules are linked by intermolecular C—H···O hydrogen bonds into head-to-tail chains along the *a* axis. The crystal packing also features C—H···$\pi$ interactions. The crystal studied was a pseudo-merohedral twin with twin law (100 0$\bar{1}$0 00$\bar{1}$) and a refined component ratio of 0.6103 (16):0.3897 (16).

## Related literature

For the preparation and applications of chalcones, see: Mori *et al.* (2003); Kumar *et al.* (2006); Amir *et al.* (2008); Atwal *et al.* (1990). For a related structure, see: Kobkeatthawin *et al.* (2011). For reference bond lengths, see: Allen *et al.* (1987). For stability of the temperature controller used in the data collection, see: Cosier & Glazer (1986).



## Experimental

### Crystal data

$C_{21}H_{18}O_2S$
$M_r$ = 334.41
Monoclinic, *Pc*
$a$ = 18.6118 (14) Å
$b$ = 15.0510 (12) Å
$c$ = 5.9227 (5) Å
$\beta$ = 90.0005 (15)°
$V$ = 1659.1 (2) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.21 mm$^{-1}$
$T$ = 100 K
0.45 × 0.10 × 0.09 mm

### Data collection

Bruker APEX DUO CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min}$ = 0.913, $T_{max}$ = 0.982
18668 measured reflections
8757 independent reflections
8185 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.041

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.136
$S$ = 1.05
8757 reflections
438 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.65 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.37 e Å$^{-3}$
Absolute structure: Flack (1983), 3893 Friedel pairs
Flack parameter: 0.24 (8)

**Table 1**
Hydrogen-bond geometry (Å, °).

*Cg*1, *Cg*2 and *Cg*3 are the centroids of the C1*A*/C2*A*/C7*A*–C10*A*, C14*A*–C19*A* and C1*B*/C2*B*/C7*B*–C10*B* rings, respectively

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C20*A*—H20*A*···O1*A*$^{i}$ | 0.96 | 2.44 | 3.381 (5) | 165 |
| C20*B*—H20*D*···O1*B*$^{i}$ | 0.96 | 2.39 | 3.252 (5) | 149 |
| C8*A*—H8*AA*···*Cg*1$^{ii}$ | 0.93 | 2.84 | 3.565 (3) | 136 |
| C3*B*—H3*BA*···*Cg*2$^{iii}$ | 0.93 | 2.74 | 3.479 (3) | 137 |
| C8*B*—H8*BA*···*Cg*3$^{iv}$ | 0.93 | 2.78 | 3.494 (3) | 134 |
| C20*A*—H20*B*···*Cg*3$^{v}$ | 0.96 | 2.63 | 3.481 (5) | 148 |

Symmetry codes: (i) $x+1, y, z$; (ii) $x, -y, z-\frac{1}{2}$; (iii) $x-1, y, z$; (iv) $x, -y+1, z+\frac{1}{2}$; (v) $x+1, y, z-1$.

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2777).

‡ Thomson Reuters ResearcherID: A-3561-2009.

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# supporting information

*Acta Cryst.* (2012). E**68**, o2277–o2278 [https://doi.org/10.1107/S1600536812028930]

## (2*E*)-3-(6-Methoxynaphthalen-2-yl)-1-[4-(methylsulfanyl)phenyl]prop-2-en-1-one

**Hoong-Kun Fun, Tze Shyang Chia, Mahesh Padaki, Arun M. Isloor and A. F. Ismail**

### S1. Comment

Chalcones are unsaturated ketones containing the reactive ketoethylenic group —CO—CH═CH—. These compounds are coloured due to the presence of the chromophore —CO—CH═CH—, and depends on the presence of other auxochromes. Several methods are available for the preparation of chalcones (Mori *et al.*, 2003; Kumar *et al.*, 2006). The most convenient method is the Claisen-Schimdt condensation of equimolar quantities of arylmethylketone with aryl aldehyde in the presence of alcoholic alkali (Amir *et al.*, 2008). Chalcones are used to synthesize several derivatives like cyanopyridines, pyrazolines, isoxazoles and pyrimidines with different heterocyclic ring systems (Atwal *et al.*, 1990). In view of the importance of chalcones, the title compound was synthesized and its crystal structure is reported herein.

The asymmetric unit of the title compound (Fig. 1) consists of two crystallographically independent molecules (*A* and *B*). The molecules exist in *trans* configuration with respect to the central C11═C12 bond. The naphthalene ring system [C1–C10; maximum deviations = 0.037 (3) and 0.041 (3) Å at atom C4 for both molecules] makes dihedral angles of 51.62 (12)° [molecule *A*] and 52.69 (12)° [molecule *B*] with the C14–C19 benzene ring. The prop-2-en-1-one group [maximum deviations = 0.0426 (23) Å at atom C13A and 0.0846 (21) Å at atom C13B] forms dihedral angles of 22.84 (15) and 29.02 (12)° with the adjacent naphthalene ring system and benzene ring, respectively in molecules *A*, whereas the corresponding angles are 30.04 (12) and 23.33 (12)° in molecule *B*. Bond lengths (Allen *et al.*, 1987) and angles are within normal ranges and are comparable to those found in a related structure (Kobkeatthawin *et al.*, 2011).

In the crystal (Fig. 2), molecules are linked by intermolecular C20A—H20A···O1A and C20B—H20D···O1B hydrogen bonds into chains in head-to-tail fashion, propagating along the *a* axis. The crystal packing is further stabilized by the C—H···$\pi$ interactions (Table 1), involving *Cg*1, *Cg*2 and *Cg*3 which are the centroids of C1A/C2A/C7A–C10A, C14A–C19A and C1B/C2B/C7B–C10B rings, respectively.

### S2. Experimental

To a thoroughly stirred solution of 6-methoxy-2-naphthaldehyde (0.5 g, 10 mmol) and 1-[4-(methylsulfanyl)phenyl]-ethanone (1.66 g, 10 mmol) in 5 ml methanol, 0.5 ml of 40% NaOH solution was added. The reaction mixture was stirred overnight and the solid separated was collected by filtration. The product obtained was recrystallized from methanol. Yield: 2.65 g, 79.3%. M.p. 459–461 K.

### S3. Refinement

All H atoms were positioned geometrically [C—H = 0.93 and 0.96 Å] and refined using a riding model with $U_{iso}$(H) = 1.2 or 1.5$U_{eq}$(C). A rotating group model was applied to the methyl groups. The crystal was a pseudo-merohedral twin with twin law (100 0$\bar{1}$0 00$\bar{1}$) and BASF of 0.3897 (16).

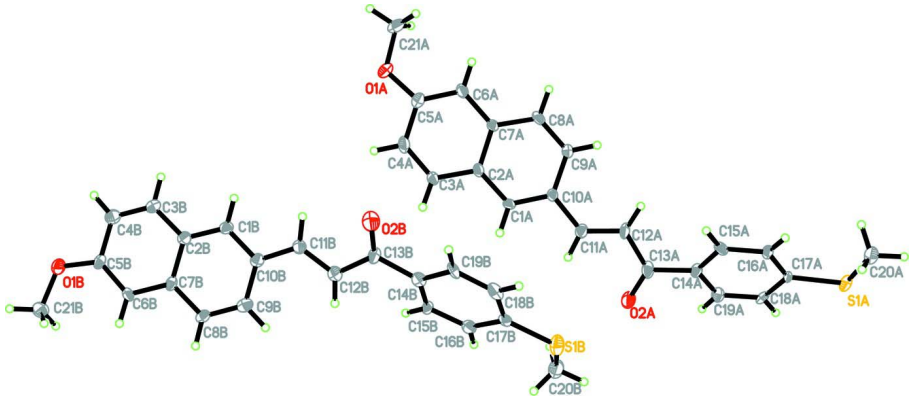


**Figure 1**

The molecular structure of the title compound with atom labels and 50% probability displacement ellipsoids.

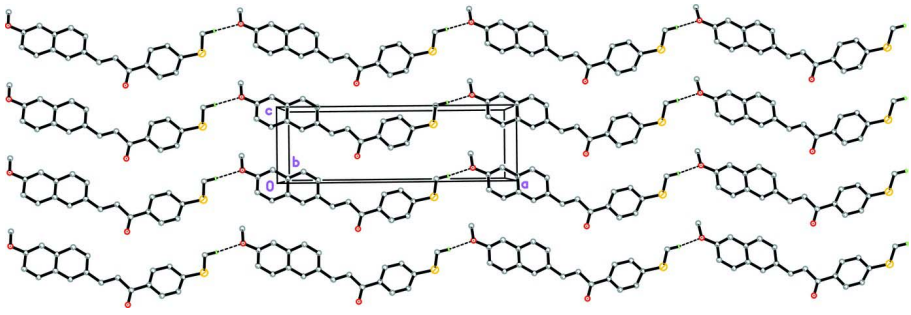


**Figure 2**

The crystal packing of the title compound. Hydrogen atoms not involved in hydrogen bonding (dashed lines) have been omitted for clarity.

### (2*E*)-3-(6-Methoxynaphthalen-2-yl)-1-[4-(methylsulfanyl)phenyl]prop- 2-en-1-one

*Crystal data*

$C_{21}H_{18}O_2S$
$M_r = 334.41$
Monoclinic, *Pc*
Hall symbol: P -2yc
$a = 18.6118\ (14)$ Å
$b = 15.0510\ (12)$ Å
$c = 5.9227\ (5)$ Å
$\beta = 90.0005\ (15)°$
$V = 1659.1\ (2)$ Å$^3$
$Z = 4$
$F(000) = 704$
$D_x = 1.339$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6635 reflections
$\theta = 2.6–29.9°$
$\mu = 0.21$ mm$^{-1}$
$T = 100$ K
Needle, yellow
0.45 × 0.10 × 0.09 mm

*Data collection*

Bruker APEX DUO CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min} = 0.913$, $T_{max} = 0.982$
18668 measured reflections
8757 independent reflections
8185 reflections with $I > 2\sigma(I)$
$R_{int} = 0.041$
$\theta_{max} = 30.1°$, $\theta_{min} = 1.7°$
$h = -26\rightarrow26$
$k = -21\rightarrow20$
$l = -8\rightarrow8$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.055$
$wR(F^2) = 0.136$
$S = 1.05$
8757 reflections
438 parameters
2 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0704P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.65$ e Å$^{-3}$
$\Delta\rho_{min} = -0.37$ e Å$^{-3}$
Absolute structure: Flack (1983), 3893 Friedel pairs
Absolute structure parameter: 0.24 (8)

*Special details*

**Experimental**. The crystal was placed in the cold stream of an Oxford Cryosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1) K.

**Geometry**. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on $F^2$, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative $F^2$. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on $F^2$ are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| S1A | 1.08822 (5) | 0.10393 (6) | 0.36728 (17) | 0.02342 (18) |
| O1A | 0.26820 (13) | 0.12565 (17) | −0.1262 (6) | 0.0267 (5) |
| O2A | 0.75451 (14) | 0.1316 (2) | 0.7822 (5) | 0.0350 (6) |
| C1A | 0.52042 (16) | 0.16767 (19) | 0.3703 (6) | 0.0150 (5) |
| H1AA | 0.5183 | 0.1960 | 0.5096 | 0.018* |
| C2A | 0.45726 (17) | 0.15987 (19) | 0.2382 (6) | 0.0155 (6) |
| C3A | 0.38979 (15) | 0.19520 (18) | 0.3088 (6) | 0.0173 (6) |
| H3AA | 0.3865 | 0.2254 | 0.4455 | 0.021* |
| C4A | 0.33029 (17) | 0.1853 (2) | 0.1788 (7) | 0.0219 (7) |
| H4AA | 0.2873 | 0.2113 | 0.2245 | 0.026* |
| C5A | 0.33241 (18) | 0.1362 (2) | −0.0252 (7) | 0.0191 (7) |
| C6A | 0.39676 (18) | 0.1015 (2) | −0.1018 (7) | 0.0180 (6) |
| H6AA | 0.3985 | 0.0702 | −0.2370 | 0.022* |
| C7A | 0.45972 (17) | 0.11400 (19) | 0.0271 (6) | 0.0136 (6) |
| C8A | 0.52828 (17) | 0.0818 (2) | −0.0451 (6) | 0.0177 (6) |
| H8AA | 0.5316 | 0.0531 | −0.1837 | 0.021* |
| C9A | 0.58886 (19) | 0.09160 (19) | 0.0813 (6) | 0.0172 (6) |
| H9AA | 0.6327 | 0.0707 | 0.0280 | 0.021* |
| C10A | 0.58450 (17) | 0.13411 (19) | 0.2960 (6) | 0.0146 (5) |
| C11A | 0.64673 (18) | 0.1402 (2) | 0.4461 (6) | 0.0194 (6) |
| H11A | 0.6372 | 0.1588 | 0.5928 | 0.023* |

| | | | | |
|---|---|---|---|---|
| C12A | 0.71575 (16) | 0.1225 (2) | 0.3995 (7) | 0.0193 (7) |
| H12A | 0.7293 | 0.1082 | 0.2528 | 0.023* |
| C13A | 0.77081 (19) | 0.1256 (2) | 0.5813 (7) | 0.0226 (7) |
| C14A | 0.84832 (17) | 0.1204 (2) | 0.5130 (7) | 0.0167 (6) |
| C15A | 0.87291 (18) | 0.1513 (2) | 0.3048 (6) | 0.0177 (6) |
| H15A | 0.8403 | 0.1730 | 0.1994 | 0.021* |
| C16A | 0.94659 (16) | 0.14992 (19) | 0.2532 (6) | 0.0157 (6) |
| H16A | 0.9633 | 0.1726 | 0.1169 | 0.019* |
| C17A | 0.99451 (15) | 0.11367 (19) | 0.4108 (6) | 0.0137 (6) |
| C18A | 0.96989 (16) | 0.08086 (19) | 0.6188 (6) | 0.0163 (6) |
| H18A | 1.0019 | 0.0559 | 0.7215 | 0.020* |
| C19A | 0.89735 (18) | 0.0861 (2) | 0.6689 (7) | 0.0182 (6) |
| H19A | 0.8810 | 0.0664 | 0.8086 | 0.022* |
| C20A | 1.1033 (2) | 0.1573 (3) | 0.0992 (7) | 0.0312 (9) |
| H20A | 1.1534 | 0.1538 | 0.0613 | 0.047* |
| H20B | 1.0891 | 0.2185 | 0.1087 | 0.047* |
| H20C | 1.0755 | 0.1281 | −0.0153 | 0.047* |
| C21A | 0.2639 (2) | 0.0665 (3) | −0.3144 (7) | 0.0290 (8) |
| H21A | 0.2150 | 0.0621 | −0.3638 | 0.044* |
| H21B | 0.2809 | 0.0088 | −0.2703 | 0.044* |
| H21C | 0.2931 | 0.0888 | −0.4354 | 0.044* |
| S1B | 0.65875 (5) | 0.38034 (6) | 0.7749 (2) | 0.0290 (2) |
| O1B | −0.17124 (13) | 0.37693 (16) | 1.1700 (5) | 0.0232 (5) |
| O2B | 0.32634 (15) | 0.40237 (17) | 0.3454 (6) | 0.0281 (6) |
| C1B | 0.08998 (19) | 0.33729 (19) | 0.7171 (6) | 0.0173 (6) |
| H1BA | 0.0896 | 0.3105 | 0.5756 | 0.021* |
| C2B | 0.02541 (17) | 0.34493 (18) | 0.8358 (6) | 0.0171 (6) |
| C3B | −0.04127 (17) | 0.31198 (19) | 0.7549 (6) | 0.0191 (6) |
| H3BA | −0.0420 | 0.2826 | 0.6168 | 0.023* |
| C4B | −0.10425 (17) | 0.3214 (2) | 0.8700 (7) | 0.0207 (6) |
| H4BA | −0.1465 | 0.2968 | 0.8142 | 0.025* |
| C5B | −0.10433 (18) | 0.3700 (2) | 1.0789 (6) | 0.0183 (6) |
| C6B | −0.04156 (17) | 0.4025 (2) | 1.1700 (6) | 0.0163 (6) |
| H6BA | −0.0422 | 0.4323 | 1.3076 | 0.020* |
| C7B | 0.02500 (17) | 0.3900 (2) | 1.0507 (6) | 0.0155 (6) |
| C8B | 0.09134 (18) | 0.41933 (19) | 1.1407 (6) | 0.0175 (6) |
| H8BA | 0.0924 | 0.4465 | 1.2817 | 0.021* |
| C9B | 0.1544 (2) | 0.4080 (2) | 1.0217 (7) | 0.0207 (7) |
| H9BA | 0.1975 | 0.4267 | 1.0855 | 0.025* |
| C10B | 0.15495 (18) | 0.36844 (18) | 0.8037 (7) | 0.0174 (7) |
| C11B | 0.21800 (18) | 0.3661 (2) | 0.6598 (6) | 0.0174 (6) |
| H11B | 0.2111 | 0.3475 | 0.5117 | 0.021* |
| C12B | 0.28628 (19) | 0.3885 (2) | 0.7199 (7) | 0.0224 (7) |
| H12B | 0.2974 | 0.4005 | 0.8699 | 0.027* |
| C13B | 0.34251 (18) | 0.3934 (2) | 0.5438 (7) | 0.0185 (7) |
| C14B | 0.41983 (19) | 0.38928 (19) | 0.6142 (7) | 0.0174 (6) |
| C15B | 0.44145 (15) | 0.35310 (19) | 0.8180 (6) | 0.0142 (6) |
| H15B | 0.4073 | 0.3326 | 0.9201 | 0.017* |

| | | | | |
|---|---|---|---|---|
| C16B | 0.51400 (18) | 0.3474 (2) | 0.8703 (7) | 0.0202 (6) |
| H16B | 0.5279 | 0.3219 | 1.0066 | 0.024* |
| C17B | 0.56853 (17) | 0.38018 (18) | 0.7174 (6) | 0.0152 (6) |
| C18B | 0.5429 (2) | 0.4159 (2) | 0.5152 (7) | 0.0220 (7) |
| H18B | 0.5763 | 0.4383 | 0.4131 | 0.026* |
| C19B | 0.47186 (17) | 0.4199 (2) | 0.4584 (6) | 0.0169 (6) |
| H19B | 0.4579 | 0.4426 | 0.3190 | 0.020* |
| C20B | 0.6682 (2) | 0.3138 (3) | 1.0244 (8) | 0.0311 (8) |
| H20D | 0.7182 | 0.3083 | 1.0618 | 0.047* |
| H20E | 0.6484 | 0.2559 | 0.9977 | 0.047* |
| H20F | 0.6432 | 0.3416 | 1.1473 | 0.047* |
| C21B | −0.17812 (19) | 0.4323 (2) | 1.3649 (7) | 0.0261 (7) |
| H21D | −0.2281 | 0.4428 | 1.3952 | 0.039* |
| H21E | −0.1544 | 0.4879 | 1.3381 | 0.039* |
| H21F | −0.1565 | 0.4033 | 1.4924 | 0.039* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1A | 0.0118 (3) | 0.0298 (4) | 0.0287 (5) | −0.0011 (3) | −0.0032 (4) | −0.0013 (4) |
| O1A | 0.0175 (11) | 0.0359 (12) | 0.0267 (14) | 0.0022 (9) | −0.0083 (13) | −0.0057 (13) |
| O2A | 0.0178 (12) | 0.0736 (19) | 0.0135 (12) | 0.0016 (12) | −0.0024 (12) | 0.0005 (15) |
| C1A | 0.0163 (12) | 0.0190 (12) | 0.0097 (13) | 0.0026 (10) | −0.0015 (13) | −0.0023 (12) |
| C2A | 0.0128 (12) | 0.0167 (12) | 0.0169 (15) | 0.0035 (10) | 0.0019 (13) | −0.0011 (12) |
| C3A | 0.0143 (12) | 0.0174 (11) | 0.0204 (15) | 0.0013 (9) | 0.0016 (12) | −0.0048 (12) |
| C4A | 0.0143 (13) | 0.0220 (14) | 0.0293 (18) | 0.0047 (11) | 0.0030 (14) | −0.0020 (14) |
| C5A | 0.0151 (15) | 0.0188 (14) | 0.0235 (17) | −0.0001 (11) | −0.0025 (14) | 0.0009 (13) |
| C6A | 0.0159 (14) | 0.0218 (14) | 0.0163 (16) | 0.0031 (11) | 0.0036 (14) | 0.0000 (12) |
| C7A | 0.0138 (14) | 0.0167 (14) | 0.0104 (13) | 0.0009 (10) | 0.0015 (13) | 0.0008 (11) |
| C8A | 0.0197 (15) | 0.0229 (14) | 0.0104 (13) | 0.0042 (11) | 0.0055 (13) | 0.0012 (11) |
| C9A | 0.0130 (12) | 0.0195 (13) | 0.0191 (15) | 0.0017 (11) | 0.0011 (14) | −0.0014 (12) |
| C10A | 0.0117 (12) | 0.0193 (12) | 0.0127 (13) | 0.0048 (10) | −0.0006 (14) | 0.0006 (12) |
| C11A | 0.0147 (14) | 0.0265 (15) | 0.0169 (16) | 0.0008 (12) | −0.0010 (14) | 0.0022 (13) |
| C12A | 0.0091 (12) | 0.0290 (15) | 0.0198 (18) | 0.0014 (10) | 0.0016 (13) | 0.0046 (14) |
| C13A | 0.0147 (15) | 0.0344 (17) | 0.0188 (17) | 0.0007 (13) | 0.0032 (14) | 0.0084 (14) |
| C14A | 0.0126 (14) | 0.0202 (14) | 0.0173 (16) | 0.0007 (11) | −0.0016 (13) | 0.0030 (12) |
| C15A | 0.0199 (14) | 0.0228 (14) | 0.0105 (14) | 0.0060 (11) | 0.0015 (13) | 0.0012 (12) |
| C16A | 0.0112 (12) | 0.0165 (12) | 0.0192 (16) | 0.0007 (9) | 0.0001 (13) | −0.0004 (12) |
| C17A | 0.0070 (11) | 0.0168 (12) | 0.0173 (17) | −0.0017 (9) | 0.0014 (12) | −0.0055 (11) |
| C18A | 0.0131 (13) | 0.0146 (12) | 0.0213 (17) | −0.0036 (10) | −0.0057 (13) | −0.0004 (11) |
| C19A | 0.0167 (14) | 0.0179 (13) | 0.0201 (15) | −0.0007 (10) | 0.0010 (14) | 0.0034 (12) |
| C20A | 0.0181 (16) | 0.048 (2) | 0.028 (2) | −0.0047 (14) | 0.0022 (16) | −0.0040 (18) |
| C21A | 0.0246 (17) | 0.0407 (19) | 0.0218 (17) | −0.0028 (15) | −0.0100 (16) | −0.0025 (16) |
| S1B | 0.0183 (4) | 0.0299 (4) | 0.0388 (6) | −0.0019 (3) | 0.0068 (4) | 0.0041 (4) |
| O1B | 0.0141 (11) | 0.0307 (12) | 0.0247 (13) | −0.0029 (9) | 0.0019 (11) | −0.0019 (11) |
| O2B | 0.0273 (13) | 0.0315 (12) | 0.0254 (15) | 0.0045 (10) | 0.0019 (13) | 0.0080 (12) |
| C1B | 0.0177 (13) | 0.0218 (13) | 0.0125 (14) | −0.0009 (12) | −0.0021 (13) | 0.0003 (11) |
| C2B | 0.0186 (14) | 0.0122 (11) | 0.0204 (17) | 0.0012 (9) | −0.0028 (14) | −0.0003 (11) |

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|---|---|---|---|---|---|---|
| C3B | 0.0189 (13) | 0.0196 (12) | 0.0187 (15) | −0.0035 (10) | −0.0036 (14) | −0.0001 (13) |
| C4B | 0.0214 (14) | 0.0189 (13) | 0.0219 (15) | −0.0035 (10) | −0.0008 (16) | 0.0003 (13) |
| C5B | 0.0110 (13) | 0.0225 (14) | 0.0214 (17) | −0.0030 (11) | −0.0009 (14) | 0.0021 (13) |
| C6B | 0.0151 (13) | 0.0182 (13) | 0.0156 (14) | 0.0030 (11) | 0.0040 (13) | −0.0014 (12) |
| C7B | 0.0117 (14) | 0.0204 (14) | 0.0145 (15) | 0.0002 (10) | −0.0008 (13) | 0.0050 (12) |
| C8B | 0.0177 (13) | 0.0172 (13) | 0.0175 (14) | −0.0005 (11) | −0.0052 (14) | 0.0012 (11) |
| C9B | 0.0228 (17) | 0.0183 (13) | 0.0211 (17) | −0.0029 (12) | −0.0049 (16) | 0.0002 (13) |
| C10B | 0.0170 (13) | 0.0121 (11) | 0.0231 (19) | −0.0016 (10) | −0.0014 (15) | −0.0009 (12) |
| C11B | 0.0176 (14) | 0.0204 (14) | 0.0141 (14) | 0.0015 (11) | −0.0002 (13) | 0.0023 (12) |
| C12B | 0.0199 (16) | 0.0271 (16) | 0.0203 (18) | 0.0008 (12) | 0.0022 (15) | −0.0018 (13) |
| C13B | 0.0133 (15) | 0.0231 (15) | 0.0192 (17) | 0.0001 (11) | −0.0005 (13) | 0.0052 (13) |
| C14B | 0.0193 (14) | 0.0121 (12) | 0.0207 (17) | −0.0030 (10) | 0.0039 (13) | −0.0002 (11) |
| C15B | 0.0106 (12) | 0.0181 (12) | 0.0140 (15) | −0.0035 (9) | 0.0017 (11) | 0.0020 (11) |
| C16B | 0.0203 (14) | 0.0214 (13) | 0.0189 (16) | −0.0018 (11) | 0.0029 (15) | −0.0034 (14) |
| C17B | 0.0187 (14) | 0.0095 (11) | 0.0176 (15) | 0.0055 (9) | −0.0008 (12) | −0.0038 (10) |
| C18B | 0.0258 (16) | 0.0164 (13) | 0.0237 (18) | 0.0012 (12) | 0.0100 (16) | −0.0005 (13) |
| C19B | 0.0188 (14) | 0.0159 (13) | 0.0161 (14) | 0.0024 (10) | 0.0094 (13) | 0.0018 (11) |
| C20B | 0.0211 (16) | 0.0379 (19) | 0.034 (2) | 0.0000 (14) | −0.0004 (17) | 0.0001 (17) |
| C21B | 0.0251 (15) | 0.0360 (17) | 0.0171 (15) | −0.0016 (13) | 0.0050 (16) | −0.0020 (16) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| S1A—C17A | 1.769 (3) | S1B—C17B | 1.713 (3) |
| S1A—C20A | 1.802 (5) | S1B—C20B | 1.794 (5) |
| O1A—C5A | 1.346 (4) | O1B—C5B | 1.361 (4) |
| O1A—C21A | 1.429 (5) | O1B—C21B | 1.429 (5) |
| O2A—C13A | 1.231 (5) | O2B—C13B | 1.220 (5) |
| C1A—C10A | 1.368 (4) | C1B—C10B | 1.395 (5) |
| C1A—C2A | 1.417 (4) | C1B—C2B | 1.397 (5) |
| C1A—H1AA | 0.9300 | C1B—H1BA | 0.9300 |
| C2A—C3A | 1.426 (4) | C2B—C3B | 1.420 (4) |
| C2A—C7A | 1.429 (5) | C2B—C7B | 1.443 (5) |
| C3A—C4A | 1.357 (5) | C3B—C4B | 1.364 (5) |
| C3A—H3AA | 0.9300 | C3B—H3BA | 0.9300 |
| C4A—C5A | 1.418 (5) | C4B—C5B | 1.437 (5) |
| C4A—H4AA | 0.9300 | C4B—H4BA | 0.9300 |
| C5A—C6A | 1.383 (5) | C5B—C6B | 1.377 (5) |
| C6A—C7A | 1.411 (5) | C6B—C7B | 1.439 (5) |
| C6A—H6AA | 0.9300 | C6B—H6BA | 0.9300 |
| C7A—C8A | 1.430 (4) | C7B—C8B | 1.415 (5) |
| C8A—C9A | 1.361 (5) | C8B—C9B | 1.379 (5) |
| C8A—H8AA | 0.9300 | C8B—H8BA | 0.9300 |
| C9A—C10A | 1.426 (5) | C9B—C10B | 1.422 (5) |
| C9A—H9AA | 0.9300 | C9B—H9BA | 0.9300 |
| C10A—C11A | 1.463 (4) | C10B—C11B | 1.451 (5) |
| C11A—C12A | 1.341 (4) | C11B—C12B | 1.362 (5) |
| C11A—H11A | 0.9300 | C11B—H11B | 0.9300 |
| C12A—C13A | 1.487 (5) | C12B—C13B | 1.479 (5) |

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|---|---|---|---|
| C12A—H12A | 0.9300 | C12B—H12B | 0.9300 |
| C13A—C14A | 1.500 (5) | C13B—C14B | 1.500 (5) |
| C14A—C15A | 1.395 (5) | C14B—C15B | 1.384 (5) |
| C14A—C19A | 1.397 (5) | C14B—C19B | 1.415 (4) |
| C15A—C16A | 1.405 (4) | C15B—C16B | 1.388 (4) |
| C15A—H15A | 0.9300 | C15B—H15B | 0.9300 |
| C16A—C17A | 1.402 (5) | C16B—C17B | 1.447 (5) |
| C16A—H16A | 0.9300 | C16B—H16B | 0.9300 |
| C17A—C18A | 1.404 (5) | C17B—C18B | 1.396 (5) |
| C18A—C19A | 1.385 (4) | C18B—C19B | 1.366 (5) |
| C18A—H18A | 0.9300 | C18B—H18B | 0.9300 |
| C19A—H19A | 0.9300 | C19B—H19B | 0.9300 |
| C20A—H20A | 0.9600 | C20B—H20D | 0.9600 |
| C20A—H20B | 0.9600 | C20B—H20E | 0.9600 |
| C20A—H20C | 0.9600 | C20B—H20F | 0.9600 |
| C21A—H21A | 0.9600 | C21B—H21D | 0.9600 |
| C21A—H21B | 0.9600 | C21B—H21E | 0.9600 |
| C21A—H21C | 0.9600 | C21B—H21F | 0.9600 |

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|---|---|---|---|
| C17A—S1A—C20A | 104.21 (17) | C17B—S1B—C20B | 105.05 (17) |
| C5A—O1A—C21A | 118.0 (3) | C5B—O1B—C21B | 116.5 (3) |
| C10A—C1A—C2A | 121.0 (3) | C10B—C1B—C2B | 122.2 (3) |
| C10A—C1A—H1AA | 119.5 | C10B—C1B—H1BA | 118.9 |
| C2A—C1A—H1AA | 119.5 | C2B—C1B—H1BA | 118.9 |
| C1A—C2A—C3A | 122.5 (3) | C1B—C2B—C3B | 123.6 (3) |
| C1A—C2A—C7A | 119.8 (3) | C1B—C2B—C7B | 119.2 (3) |
| C3A—C2A—C7A | 117.7 (3) | C3B—C2B—C7B | 117.2 (3) |
| C4A—C3A—C2A | 120.8 (3) | C4B—C3B—C2B | 123.1 (3) |
| C4A—C3A—H3AA | 119.6 | C4B—C3B—H3BA | 118.4 |
| C2A—C3A—H3AA | 119.6 | C2B—C3B—H3BA | 118.4 |
| C3A—C4A—C5A | 121.2 (3) | C3B—C4B—C5B | 119.0 (3) |
| C3A—C4A—H4AA | 119.4 | C3B—C4B—H4BA | 120.5 |
| C5A—C4A—H4AA | 119.4 | C5B—C4B—H4BA | 120.5 |
| O1A—C5A—C6A | 125.4 (4) | O1B—C5B—C6B | 126.4 (3) |
| O1A—C5A—C4A | 114.6 (3) | O1B—C5B—C4B | 112.4 (3) |
| C6A—C5A—C4A | 120.0 (3) | C6B—C5B—C4B | 121.2 (3) |
| C5A—C6A—C7A | 119.4 (3) | C5B—C6B—C7B | 119.5 (3) |
| C5A—C6A—H6AA | 120.3 | C5B—C6B—H6BA | 120.3 |
| C7A—C6A—H6AA | 120.3 | C7B—C6B—H6BA | 120.3 |
| C6A—C7A—C2A | 120.7 (3) | C8B—C7B—C6B | 121.7 (3) |
| C6A—C7A—C8A | 122.3 (3) | C8B—C7B—C2B | 118.3 (3) |
| C2A—C7A—C8A | 117.0 (3) | C6B—C7B—C2B | 120.0 (3) |
| C9A—C8A—C7A | 122.5 (3) | C9B—C8B—C7B | 120.8 (3) |
| C9A—C8A—H8AA | 118.7 | C9B—C8B—H8BA | 119.6 |
| C7A—C8A—H8AA | 118.7 | C7B—C8B—H8BA | 119.6 |
| C8A—C9A—C10A | 119.5 (3) | C8B—C9B—C10B | 121.4 (3) |
| C8A—C9A—H9AA | 120.3 | C8B—C9B—H9BA | 119.3 |
| C10A—C9A—H9AA | 120.3 | C10B—C9B—H9BA | 119.3 |

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|---|---|---|---|
| C1A—C10A—C9A | 120.1 (3) | C1B—C10B—C9B | 117.9 (3) |
| C1A—C10A—C11A | 118.2 (3) | C1B—C10B—C11B | 118.5 (3) |
| C9A—C10A—C11A | 121.7 (3) | C9B—C10B—C11B | 123.3 (3) |
| C12A—C11A—C10A | 128.4 (4) | C12B—C11B—C10B | 126.5 (3) |
| C12A—C11A—H11A | 115.8 | C12B—C11B—H11B | 116.7 |
| C10A—C11A—H11A | 115.8 | C10B—C11B—H11B | 116.7 |
| C11A—C12A—C13A | 120.3 (4) | C11B—C12B—C13B | 119.2 (4) |
| C11A—C12A—H12A | 119.8 | C11B—C12B—H12B | 120.4 |
| C13A—C12A—H12A | 119.8 | C13B—C12B—H12B | 120.4 |
| O2A—C13A—C12A | 122.2 (3) | O2B—C13B—C12B | 120.6 (3) |
| O2A—C13A—C14A | 120.1 (3) | O2B—C13B—C14B | 120.6 (3) |
| C12A—C13A—C14A | 117.8 (3) | C12B—C13B—C14B | 118.7 (3) |
| C15A—C14A—C19A | 119.5 (3) | C15B—C14B—C19B | 119.9 (3) |
| C15A—C14A—C13A | 122.5 (3) | C15B—C14B—C13B | 122.5 (3) |
| C19A—C14A—C13A | 118.0 (3) | C19B—C14B—C13B | 117.5 (3) |
| C14A—C15A—C16A | 120.5 (3) | C14B—C15B—C16B | 120.1 (3) |
| C14A—C15A—H15A | 119.7 | C14B—C15B—H15B | 119.9 |
| C16A—C15A—H15A | 119.7 | C16B—C15B—H15B | 119.9 |
| C17A—C16A—C15A | 118.8 (3) | C15B—C16B—C17B | 121.4 (3) |
| C17A—C16A—H16A | 120.6 | C15B—C16B—H16B | 119.3 |
| C15A—C16A—H16A | 120.6 | C17B—C16B—H16B | 119.3 |
| C16A—C17A—C18A | 120.9 (3) | C18B—C17B—C16B | 115.4 (3) |
| C16A—C17A—S1A | 124.2 (3) | C18B—C17B—S1B | 120.3 (3) |
| C18A—C17A—S1A | 114.9 (2) | C16B—C17B—S1B | 124.3 (3) |
| C19A—C18A—C17A | 119.1 (3) | C19B—C18B—C17B | 124.0 (3) |
| C19A—C18A—H18A | 120.5 | C19B—C18B—H18B | 118.0 |
| C17A—C18A—H18A | 120.5 | C17B—C18B—H18B | 118.0 |
| C18A—C19A—C14A | 121.1 (3) | C18B—C19B—C14B | 119.2 (3) |
| C18A—C19A—H19A | 119.5 | C18B—C19B—H19B | 120.4 |
| C14A—C19A—H19A | 119.5 | C14B—C19B—H19B | 120.4 |
| S1A—C20A—H20A | 109.5 | S1B—C20B—H20D | 109.5 |
| S1A—C20A—H20B | 109.5 | S1B—C20B—H20E | 109.5 |
| H20A—C20A—H20B | 109.5 | H20D—C20B—H20E | 109.5 |
| S1A—C20A—H20C | 109.5 | S1B—C20B—H20F | 109.5 |
| H20A—C20A—H20C | 109.5 | H20D—C20B—H20F | 109.5 |
| H20B—C20A—H20C | 109.5 | H20E—C20B—H20F | 109.5 |
| O1A—C21A—H21A | 109.5 | O1B—C21B—H21D | 109.5 |
| O1A—C21A—H21B | 109.5 | O1B—C21B—H21E | 109.5 |
| H21A—C21A—H21B | 109.5 | H21D—C21B—H21E | 109.5 |
| O1A—C21A—H21C | 109.5 | O1B—C21B—H21F | 109.5 |
| H21A—C21A—H21C | 109.5 | H21D—C21B—H21F | 109.5 |
| H21B—C21A—H21C | 109.5 | H21E—C21B—H21F | 109.5 |

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|---|---|---|---|
| C10A—C1A—C2A—C3A | −179.0 (3) | C10B—C1B—C2B—C3B | −178.4 (3) |
| C10A—C1A—C2A—C7A | 1.9 (5) | C10B—C1B—C2B—C7B | 2.9 (4) |
| C1A—C2A—C3A—C4A | −179.1 (3) | C1B—C2B—C3B—C4B | −178.6 (3) |
| C7A—C2A—C3A—C4A | 0.0 (5) | C7B—C2B—C3B—C4B | 0.2 (4) |
| C2A—C3A—C4A—C5A | 3.0 (5) | C2B—C3B—C4B—C5B | 2.6 (5) |

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|---|---|---|---|
| C21A—O1A—C5A—C6A | 7.0 (5) | C21B—O1B—C5B—C6B | 8.0 (5) |
| C21A—O1A—C5A—C4A | −171.2 (3) | C21B—O1B—C5B—C4B | −173.4 (3) |
| C3A—C4A—C5A—O1A | 174.6 (3) | C3B—C4B—C5B—O1B | 177.6 (3) |
| C3A—C4A—C5A—C6A | −3.7 (5) | C3B—C4B—C5B—C6B | −3.7 (5) |
| O1A—C5A—C6A—C7A | −176.9 (3) | O1B—C5B—C6B—C7B | −179.5 (3) |
| C4A—C5A—C6A—C7A | 1.2 (5) | C4B—C5B—C6B—C7B | 1.9 (5) |
| C5A—C6A—C7A—C2A | 1.8 (5) | C5B—C6B—C7B—C8B | −177.7 (3) |
| C5A—C6A—C7A—C8A | −178.4 (3) | C5B—C6B—C7B—C2B | 0.9 (4) |
| C1A—C2A—C7A—C6A | 176.7 (3) | C1B—C2B—C7B—C8B | −4.5 (4) |
| C3A—C2A—C7A—C6A | −2.4 (4) | C3B—C2B—C7B—C8B | 176.7 (3) |
| C1A—C2A—C7A—C8A | −3.1 (4) | C1B—C2B—C7B—C6B | 176.9 (3) |
| C3A—C2A—C7A—C8A | 177.8 (3) | C3B—C2B—C7B—C6B | −2.0 (4) |
| C6A—C7A—C8A—C9A | −178.2 (3) | C6B—C7B—C8B—C9B | −178.9 (3) |
| C2A—C7A—C8A—C9A | 1.7 (5) | C2B—C7B—C8B—C9B | 2.5 (4) |
| C7A—C8A—C9A—C10A | 1.1 (5) | C7B—C8B—C9B—C10B | 1.3 (5) |
| C2A—C1A—C10A—C9A | 0.9 (5) | C2B—C1B—C10B—C9B | 0.8 (4) |
| C2A—C1A—C10A—C11A | −176.8 (3) | C2B—C1B—C10B—C11B | −173.7 (3) |
| C8A—C9A—C10A—C1A | −2.4 (5) | C8B—C9B—C10B—C1B | −3.0 (5) |
| C8A—C9A—C10A—C11A | 175.2 (3) | C8B—C9B—C10B—C11B | 171.3 (3) |
| C1A—C10A—C11A—C12A | −170.7 (3) | C1B—C10B—C11B—C12B | −175.7 (3) |
| C9A—C10A—C11A—C12A | 11.6 (5) | C9B—C10B—C11B—C12B | 10.1 (5) |
| C10A—C11A—C12A—C13A | −174.9 (3) | C10B—C11B—C12B—C13B | −172.1 (3) |
| C11A—C12A—C13A—O2A | 10.5 (6) | C11B—C12B—C13B—O2B | 20.4 (5) |
| C11A—C12A—C13A—C14A | −169.9 (3) | C11B—C12B—C13B—C14B | −160.9 (3) |
| O2A—C13A—C14A—C15A | −151.5 (4) | O2B—C13B—C14B—C15B | −159.8 (3) |
| C12A—C13A—C14A—C15A | 28.9 (5) | C12B—C13B—C14B—C15B | 21.5 (5) |
| O2A—C13A—C14A—C19A | 26.2 (5) | O2B—C13B—C14B—C19B | 17.0 (5) |
| C12A—C13A—C14A—C19A | −153.3 (3) | C12B—C13B—C14B—C19B | −161.7 (3) |
| C19A—C14A—C15A—C16A | −1.5 (5) | C19B—C14B—C15B—C16B | 0.4 (4) |
| C13A—C14A—C15A—C16A | 176.3 (3) | C13B—C14B—C15B—C16B | 177.1 (3) |
| C14A—C15A—C16A—C17A | 2.6 (5) | C14B—C15B—C16B—C17B | 1.2 (5) |
| C15A—C16A—C17A—C18A | −1.3 (5) | C15B—C16B—C17B—C18B | −1.1 (4) |
| C15A—C16A—C17A—S1A | 177.9 (2) | C15B—C16B—C17B—S1B | 176.8 (2) |
| C20A—S1A—C17A—C16A | 4.3 (3) | C20B—S1B—C17B—C18B | −171.2 (3) |
| C20A—S1A—C17A—C18A | −176.4 (2) | C20B—S1B—C17B—C16B | 11.0 (3) |
| C16A—C17A—C18A—C19A | −1.1 (4) | C16B—C17B—C18B—C19B | −0.7 (4) |
| S1A—C17A—C18A—C19A | 179.6 (2) | S1B—C17B—C18B—C19B | −178.7 (3) |
| C17A—C18A—C19A—C14A | 2.3 (5) | C17B—C18B—C19B—C14B | 2.2 (5) |
| C15A—C14A—C19A—C18A | −1.0 (5) | C15B—C14B—C19B—C18B | −2.1 (5) |
| C13A—C14A—C19A—C18A | −178.8 (3) | C13B—C14B—C19B—C18B | −179.0 (3) |

*Hydrogen-bond geometry (Å, º)*

Cg1, Cg2 and Cg3 are the centroids of the C1A/C2A/C7A–C10A, C14A–C19A and C1B/C2B/C7B–C10B rings, respectively

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C20*A*—H20*A*···O1*A*$^{i}$ | 0.96 | 2.44 | 3.381 (5) | 165 |
| C20*B*—H20*D*···O1*B*$^{i}$ | 0.96 | 2.39 | 3.252 (5) | 149 |
| C8*A*—H8*AA*···*Cg*1$^{ii}$ | 0.93 | 2.84 | 3.565 (3) | 136 |

| | | | | |
|---|---|---|---|---|
| C3*B*—H3*BA*···*Cg*2$^{iii}$ | 0.93 | 2.74 | 3.479 (3) | 137 |
| C8*B*—H8*BA*···*Cg*3$^{iv}$ | 0.93 | 2.78 | 3.494 (3) | 134 |
| C20*A*—H20*B*···*Cg*3$^{v}$ | 0.96 | 2.63 | 3.481 (5) | 148 |

Symmetry codes: (i) $x+1, y, z$; (ii) $x, -y, z-1/2$; (iii) $x-1, y, z$; (iv) $x, -y+1, z+1/2$; (v) $x+1, y, z-1$.